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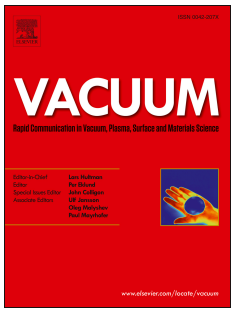

Adsorption of 2, 3, 7, 8-tetrachlorodibenzo-p-dioxin (TCDD) on pristine, defected and Al-doped carbon nanotube: A dispersion corrected DFT study

Z. Izakmehri, M. Darvish Ganji, M. Ardjmand

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Adsorption of 2, 3, 7, 8-Tetrachlorodibenzo-p-dioxin (TCDD) on pristine, defected and Al-doped carbon nanotube: A dispersion corrected DFT study

Z. Izakmehri [a], M. Darvish Ganji [b,] * and, M. Ardjmand [c]

[a] Department of Chemical Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran

[b] Department of Nanochemistry, Faculty of Pharmaceutical Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran - Iran (IAUPS)

[c] Chemical Engineering Department, Islamic Azad University, South Tehran Branch, Tehran, Iran

* Corresponding author. E-mail address: ganji_md@yahoo.com (M.D. Ganji).

Abstract:

The effective enrichment and detection of organic pollutants in the environment has been attracted much attention because of enormous concerns about human health. Using dispersion-corrected density functional theory (DFT-D2), the interactions between 2, 3, 7, 8-tetrachlorodibenzo-p-dioxin (TCDD) and pristine, defected and Al-doped carbon nanotubes (Al-CNT) were studied. The TCDD molecule was physisorbed on a pure CNT and CNT contain defects with binding energies of about -0.52 eV and -0.34 eV, respectively. The accuracy of our method was validated by hybrid B3LYP levels of theory and it was shown that there is a worthy agreement between two respected methods. However, the binding energy rises to -0.85 eV when TCDD binds to Al-CNT. The increase in binding energy is due to charge transfer from the